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Remarks on the structure-preserving finite difference scheme for the Falk model of shape memory alloys

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Abstract

In [6] and [8] the author studied the structure-preserving finite difference scheme for the Falk model which is a thermoelastic system describing the phase transition occurring in shape memory alloys, by using well-known transformation to first order system with respect to time variable. We give several scheme without the transformation for these results in order to apply the theory to multi-dimensional problems. Here we only give the basic idea and remarks. Precise proof and extended results will be given in [5].

1 Introduction

We study the following thermoelastic system:

$$\partial_t^2 u + \partial_x^4 u = \partial_x \{F_2'(\partial_x u) + \theta F_1'(\partial_x u)\}, \quad (1.1)$$

$$\partial_t \theta - \partial_x^2 \theta = \theta F_1'(\partial_x u) \partial_x \partial_t u, \quad x \in (0, L), \quad t \in (0, T], \quad (1.2)$$

$$\begin{aligned} u(t, 0) = u(t, L) = \partial_x^2 u(t, 0) = \partial_x^2 u(t, L) = \partial_x \theta(t, 0) \\ = \partial_x \theta(t, L) = 0, \quad t \in [0, T], \end{aligned} \quad (1.3)$$

$$u(0, x) = u_0(x), \quad \partial_t u(0, x) = u_1(x), \quad \theta(0, x) = \theta_0(x), \quad x \in (0, L), \quad (1.4)$$

where u and θ are the displacement and absolute temperature respectively, and the positive constant θ_c represents a critical temperature of the phase transition. This model called the Falk model represents the phase transition on lattice structure of alloy. We normalize all physical parameters without θ_c by unity. For the physical background of the model we refer the reader to [1, Chapter 5]. If we set the energy

E and the entropy S as follows:

$$E(u, \theta) := \frac{1}{2} \int_0^L |\partial_x^2 u|^2 dx + \frac{1}{2} \int_0^L |\partial_t u|^2 dx + \int_0^L F_2(\partial_x u) dx + \int_0^L \theta dx,$$

$$S(u, \theta) := \int_0^L (\log \theta - F_1(\partial_x u)) dx,$$

we can easily check that the smooth solution of the system (1.1)-(1.3) satisfies the energy conservation law and the law of increasing entropy:

$$\frac{d}{dt} E(u(t), v(t), \theta(t)) = 0, \quad \frac{d}{dt} S(u(t), \theta(t)) = \int_0^L \left| \frac{\partial_x \theta}{\theta} \right|^2 \geq 0. \quad (1.5)$$

where the latter one holds under the assumption $\theta > 0$.

Recently in [6] the author proposes a new finite difference scheme which satisfies the discrete version of (1.5) and gives existence result of solution, and in [8] the error estimate and another existence result of solution are shown by applying the energy method given in [7]. In these results ([6], [8]) the author use the well-known transformation (see e.g. [4]), namely he study the following 1st order system:

$$\begin{aligned} \partial_t w &= \partial_x^2 v, \\ \partial_t v &= -\partial_x^2 w + F_2'(w) + \theta F_1'(w), \\ \partial_t \theta &= \partial_x^2 \theta + \theta F_1'(w) \partial_x v, \end{aligned}$$

for a shear strain $w := \partial_x u$ and velocity potential v . However, when we consider the multi-dimensional case, it seems to be difficult to extend directly. Indeed, shear strain w in 1-dimensional case is no longer scalar but tensor valued in multi-dimensional cases. Then we propose here the simple new schemes by applying the result in [2] to the scheme for the original second order system (1.1)-(1.2). One of these schemes is enable to prove the existence of solution and error estimate in a similar manner to the previous result [8] though we need several modifications. Here we only give an idea of the proofs of existence and error estimate.

We will introduce two new structure-preserving numerical schemes for (1.1)-(1.2) in Section 2. The idea of outline of proofs of error estimate and existence of solution will be given in Sections 3. The precise explanation and their extended results including the results will be submitted to another journal as [5].

2 Structure-Preserving Schemes

We denote by ∂_t and ∂_x partial differential operators with respect to variables t and x , respectively. We split space interval $[0, L]$ into K -th parts and time interval $[0, T]$ into N -th parts, and hence the following relations hold $L = K\Delta x$ and $T = N\Delta t$. For $k = 0, 1, \dots, K$ and $n = 0, 1, \dots, N$ we write $u_k^{(n)} = u(k\Delta x, n\Delta t)$,

$v_k^{(n)} = v(k\Delta x, n\Delta t)$ and $\theta_k^{(n)} = \theta(k\Delta x, n\Delta t)$, for short. Let $(U_k^{(n)}, V_k^{(n)}, \Theta_k^{(n)})$ be an approximate solution corresponding to the solution $(u_k^{(n)}, v_k^{(n)}, \theta_k^{(n)})$. Let us define difference operators by

$$\begin{aligned}\delta_k^{(2)} U_k^{(n)} &:= \frac{U_{k+1}^{(n)} - 2U_k^{(n)} + U_{k-1}^{(n)}}{\Delta x^2}, & \delta_k^{(1)} U_k^{(n)} &:= \frac{U_{k+1}^{(n)} - U_{k-1}^{(n)}}{2\Delta x}, \\ \delta_k^+ U_k &:= \frac{U_{k+1} - U_k}{\Delta x}, & \delta_k^- U_k &:= \frac{U_k - U_{k-1}}{\Delta x},\end{aligned}$$

and δ_n^+ , δ_n^- , $\delta_n^{(1)}$ and $\delta_n^{(2)}$ are defined the same manner by replacing space-variable k and Δx to time-variable n and Δt . We will also use the following difference operator

$$\delta_n^{(2+)} U_k^{(n)} := \frac{U_k^{(n+2)} - U_k^{(n+1)} - U_k^{(n)} + U_k^{(n-1)}}{2\Delta t^2}$$

We approximate an integral by the trapezoidal rule

$$\sum_{k=0}^K {}'' U_k \Delta x := \left(\frac{1}{2} U_0 + \sum_{k=1}^{K-1} U_k + \frac{1}{2} U_K \right) \Delta x.$$

For these approximations the summation by parts formula:

$$\begin{aligned}\sum_{k=0}^K {}'' \left(\delta_k^{(2)} U_k \right) V_k \Delta x &= - \sum_{k=0}^K {}'' \frac{(\delta_k^+ U_k) (\delta_k^+ V_k) + (\delta_k^- U_k) (\delta_k^- V_k)}{2} \Delta x \\ &= \sum_{k=0}^K {}'' U_k \left(\delta_k^{(2)} V_k \right) \Delta x\end{aligned}\tag{2.1}$$

plays an important role in DVDm, which holds under suitable boundary condition such as

$$U_0 = \delta_k^{(2)} U_0 = V_K = \delta_k^{(2)} V_K = 0.\tag{2.2}$$

Indeed, according to Proposition 3.3 in [3], we have

$$\begin{aligned}\sum_{k=0}^K {}'' \left(\delta_k^{(2)} U_k \right) V_k \Delta x &+ \sum_{k=0}^K {}'' \frac{(\delta_k^+ U_k) (\delta_k^+ V_k) + (\delta_k^- U_k) (\delta_k^- V_k)}{2} \Delta x \\ &= \left[\frac{\delta_k^+ U_k \cdot \frac{V_{k+1} + V_k}{2} + \delta_k^- U_k \cdot \frac{V_{k-1} + V_k}{2}}{2} \right]_0^K\end{aligned}$$

From (2.2) we see several facts such as

$$U_{-1} = -U_1, \quad U_{K-1} = U_{K+1}, \quad V_{-1} = -V_1, \quad V_{K-1} = V_{K+1}.$$

Then the boundary term vanishes, namely, we complete the proof of (2.1). Similarly, it follows that under (2.2)

$$\sum_{k=0}^K \frac{(\delta_k^+ U_k)(\delta_k^+ V_k) + (\delta_k^- U_k)(\delta_k^- V_k)}{2} \Delta x = \sum_{k=0}^{K-1} \delta_k^+ U_k \delta_k^+ V_k \Delta x.$$

For a smooth function $F = F(U)$, the *difference quotient* $\partial F / \partial(U, V)$ of F is defined by

$$\frac{\partial F}{\partial(U, V)} := \begin{cases} \frac{F(U) - F(V)}{U - V}, & U \neq V, \\ F'(U), & U = V. \end{cases}$$

For example in the case $F(U) = \frac{1}{p+1} U^{p+1}$ the difference quotient of F is

$$\frac{\partial F}{\partial(U, V)} = \frac{1}{p+1} \sum_{j=0}^p U^j V^{p-j}$$

from the easy calculation. For more precise information about the difference quotient we refer to [7]. From now on, we give two schemes which are derived by applying the idea given in [2] easily.

2.1 Semi-Explicit Scheme

The first scheme is so-called semi-explicit scheme:

$$\delta_n^{(2+)} U_k^{(n)} + (\delta_k^{(2)})^2 \left(\frac{U_k^{(n+1)} + U_k^{(n)}}{2} \right) = N_{1,k}, \quad (2.3)$$

$$\delta_n^+ \Theta_k^{(n)} - \delta_k^{(2)} \Theta_k^{(n+1)} = N_{2,k}, \quad k = 0, 1, \dots, K, \quad (2.4)$$

with the boundary conditions corresponding to (1.3):

$$U_0^{(n)} = U_K^{(n)} = \delta_k^{(2)} U_0^{(n)} = \delta_k^{(2)} U_K^{(n)} = \delta_k^{(1)} \Theta_0^{(n)} = \delta_k^{(1)} \Theta_K^{(n)} = 0. \quad (2.5)$$

Here we define $N_{i,k} = N_{i,k}(U^{(n+1)}, U^{(n)}, \Theta^{(n+1)})$ ($i = 1, 2$) by

$$\begin{aligned} N_{1,k} &:= \frac{\delta_k^+}{2} \left(\frac{\partial F_2}{\partial(\delta_k^- U_k^{(n+1)}, \delta_k^- U_k^{(n)})} + \Theta_k^{(n+1)} \frac{\partial F_1}{\partial(\delta_k^- U_k^{(n+1)}, \delta_k^- U_k^{(n)})} \right) \\ &\quad + \frac{\delta_k^-}{2} \left(\frac{\partial F_2}{\partial(\delta_k^+ U_k^{(n+1)}, \delta_k^+ U_k^{(n)})} + \Theta_k^{(n+1)} \frac{\partial F_1}{\partial(\delta_k^+ U_k^{(n+1)}, \delta_k^+ U_k^{(n)})} \right), \\ N_{2,k} &:= \frac{\Theta_k^{(n+1)}}{2} \left(\frac{\partial F_1}{\partial(\delta_k^- U_k^{(n+1)}, \delta_k^- U_k^{(n)})} \delta_n^+ \delta_k^- U_k^{(n)} + \frac{\partial F_1}{\partial(\delta_k^+ U_k^{(n+1)}, \delta_k^+ U_k^{(n-1)})} \delta_n^+ \delta_k^+ U_k^{(n)} \right), \end{aligned}$$

Let the discrete energy $E_d = E_d(\mathbf{U}^{(n+1)}, \mathbf{U}^{(n)}, \mathbf{U}^{(n-1)}, \boldsymbol{\Theta}^{(n)})$ be defined by

$$E_d := \frac{1}{2} \sum_{k=0}^K {}''\delta_n^+ U_k^{(n)} \delta_n^- U_k^{(n)} \Delta x + \sum_{k=0}^K {}''\bar{F}_{2,k}(DU) \Delta x + \sum_{k=0}^K {}''\Theta_k^{(n)} \Delta x,$$

where for $i = 1, 2$ we set

$$\bar{F}_{i,k}(DU) = \frac{F_i(\delta_k^+ U_k) + F_i(\delta_k^- U_k)}{2}.$$

Then the following conservation law

$$\delta_n^+ E_d(\mathbf{U}^{(n+1)}, \mathbf{U}^{(n)}, \mathbf{U}^{(n-1)}, \boldsymbol{\Theta}^{(n)}) = 0$$

holds. Let the discrete entropy $S_d(\mathbf{U}, \boldsymbol{\Theta})$ be defined by

$$S_d(\mathbf{U}, \boldsymbol{\Theta}) := \sum_{k=0}^K {}''\{\log \Theta_k - \bar{F}_{1,k}(DU)\} \Delta x.$$

Under the assumptions of positivity of temperature, the following increasing law:

$$\delta_n^+ S_d(\mathbf{U}^{(n)}, \boldsymbol{\Theta}^{(n)}) \geq 0$$

holds. We can check these easily in the same fashion as the proofs in [6].

2.2 Implicit Scheme

The other is implicit scheme:

$$\delta_n^{(2)} U_k^{(n)} + (\delta_k^{(2)})^2 \left(\frac{U_k^{(n+1)} + U_k^{(n-1)}}{2} \right) = \tilde{N}_{1,k}, \quad (2.6)$$

$$\delta_n^+ \Theta_k^{(n)} - \delta_k^{(2)} \Theta_k^{(n+1)} = \tilde{N}_{2,k}, \quad k = 0, 1, \dots, K, \quad (2.7)$$

where

$$\begin{aligned} \tilde{N}_{1,k} &:= \frac{\delta_k^+}{2} \left(\frac{\partial F_2}{\partial(\delta_k^- U_k^{(n+1)}, \delta_k^- U_k^{(n-1)})} + \Theta_k^{(n+1)} \frac{\partial F_1}{\partial(\delta_k^- U_k^{(n+1)}, \delta_k^- U_k^{(n-1)})} \right) \\ &\quad + \frac{\delta_k^-}{2} \left(\frac{\partial F_2}{\partial(\delta_k^+ U_k^{(n+1)}, \delta_k^+ U_k^{(n-1)})} + \Theta_k^{(n+1)} \frac{\partial F_1}{\partial(\delta_k^+ U_k^{(n+1)}, \delta_k^+ U_k^{(n-1)})} \right), \\ \tilde{N}_{2,k} &:= \frac{\Theta_k^{(n+1)}}{2} \left(\frac{\partial F_1}{\partial(\delta_k^- U_k^{(n+1)}, \delta_k^- U_k^{(n-1)})} \delta_n^{(1)} \delta_k^- U_k^{(n)} + \frac{\partial F_1}{\partial(\delta_k^+ U_k^{(n+1)}, \delta_k^+ U_k^{(n-1)})} \delta_n^{(1)} \delta_k^+ U_k^{(n)} \right), \end{aligned}$$

with the boundary conditions (2.5).

Let the discrete energy and the discrete entropy be defined by

$$E_d(\mathbf{U}^{(n)}, \mathbf{U}^{(n-1)}, \boldsymbol{\Theta}^{(n)}) := \frac{1}{2} \sum_{k=0}^K \|\delta_k^- \mathbf{U}^{(n)}\|^2 \Delta x + \frac{1}{2} \sum_{k=0}^K \|\delta_k^{(2)} \mathbf{U}^{(n)}\|^2 \Delta x + \sum_{k=0}^K \|\Theta_k^{(n)}\| \Delta x$$

$$+ \sum_{k=0}^K \|\tilde{F}_{2,k}(\mathbf{DU}^{(n)}, \mathbf{DU}^{(n-1)})\| \Delta x,$$

$$S_d(\mathbf{U}^{(n)}, \mathbf{U}^{(n-1)}, \boldsymbol{\Theta}^{(n)}) := \sum_{k=0}^K \left(\log \Theta_k^{(n)} - \tilde{F}_{1,k}(\mathbf{DU}^{(n)}, \mathbf{DU}^{(n-1)}) \right) \Delta x,$$

where for $i = 1, 2$

$$\tilde{F}_{i,k}(\mathbf{DU}, \mathbf{DV}) = \frac{F_i(\delta_k^+ U_k) + F_i(\delta_k^- U_k) + F_i(\delta_k^+ V_k) + F_i(\delta_k^- V_k)}{4}.$$

Then it is easily seen that for any $n \in \mathbb{N}$ conservation law:

$$\delta_n^+ E_d(\mathbf{U}^{(n)}, \mathbf{U}^{(n-1)}, \boldsymbol{\Theta}^{(n)}) = 0,$$

and under the assumptions of positivity of temperature, the increasing law:

$$\delta_n^+ S_d(\mathbf{U}^{(n)}, \mathbf{U}^{(n-1)}, \boldsymbol{\Theta}^{(n)}) \geq 0$$

hold.

3 Existence and Error Estimate

The semi-explicit scheme is uncoupled scheme. Then when we solve (2.3), $\mathbf{U}^{(n+2)}$ can be obtained explicitly. However for the scheme the bounded-from-below of the first term in the energy (kinetic energy term) is not assured. Then the energy method given in [7] and [8] can not be applied directly. On the other hand, we can easily apply the method to the implicit scheme (2.6)-(2.7). Here we only give a remark about the fact. Before stating the mathematical results we give some definition and notation. We have used the expression in bold print to denote vectors such as $\mathbf{U} := (U_k)_{k=0}^K$, $\mathbf{V} := (V_k)_{k=0}^K$ and $\boldsymbol{\Theta} := (\Theta_k)_{k=0}^K$. Let us give a definition of several norms by

$$\|\mathbf{U}\|_{L_d^p} := \begin{cases} \left(\sum_{k=0}^K \|U_k\|^p \Delta x \right)^{\frac{1}{p}}, & p \in [1, \infty), \\ \max_{k=0,1,\dots,K} |U_k|, & p = \infty, \end{cases} \quad \|\mathbf{DU}\| := \sqrt{\sum_{k=0}^{K-1} \|\delta_k^+ U_k\|^2 \Delta x}.$$

Moreover we define the discrete Sobolev norm by

$$\|\mathbf{U}\|_{H_d^1} := \sqrt{\|\mathbf{U}\|_{L_d^2}^2 + \|\mathbf{DU}\|^2}.$$

We obtain the following results. The first theorem is related with the existence of the implicit scheme (2.6)-(2.7).

Theorem 3.1 (Existence of solution). *Suppose that $\Theta_k^{(0)} \geq 0$ for $k = 0, 1, \dots, K$. For sufficient small Δt there exists a unique global solution $(\mathbf{U}^{(n)}, \mathbf{V}^{(n)}, \Theta^{(n)})$ ($n = 1, 2, \dots, N$) for the scheme (2.6)-(2.7) with (2.5) satisfying $\Theta_k^{(n)} \geq 0$ for $k = 0, 1, \dots, K$.*

We can also show the error estimate. Let us denote

$$e_{u,k}^{(n)} = U_k^{(n)} - u_k^{(n)}, \quad e_{v,k}^{(n)} = V_k^{(n)} - v_k^{(n)}, \quad e_{\theta,k}^{(n)} = \Theta_k^{(n)} - \theta_k^{(n)}.$$

Theorem 3.2 (Error estimate). *Assume that (u, v, θ) is a smooth solution for (1.1)-(1.4) satisfying $(u, v, \theta) \in L^\infty([0, T], H^3 \times H^3 \times H^3)$ and $(\partial_t u, \partial_t v, \partial_t \theta) \in L^\infty([0, T], H^3 \times H^3 \times H^1)$, and denote the bounds by*

$$\|\mathbf{U}^{(n)}\|_{H_d^1}, \|\mathbf{V}^{(n)}\|_{H_d^1}, \|\mathbf{u}^{(n)}\|_{H_d^1}, \|\mathbf{v}^{(n)}\|_{H_d^1}, \|\boldsymbol{\theta}^{(n)}\|_{H_d^1} \leq C_1.$$

Then there exists a constant $C_{err} = C_{err}(C_1)$ such that for $\Delta t < 1/C_{err}$

$$\|e_u^{(n)}\|_{H_d^1} + \|e_v^{(n)}\|_{H_d^1} + \|e_\theta^{(n)}\|_{L_d^2} \leq C(\Delta t + \Delta x^2).$$

We prove these theorems in similar manner to the proofs of [8] with small modification. The key estimate of the modification is the following type of Sobolev inequality which is well-known in the continuous case. More precisely we will give exact proofs in [5].

Proposition 3.3 (Sobolev inequality). *Assume that $U_k = \delta_k^{(2)} U_k = 0$ on $k = 0, K$. It holds that*

$$\left\| \delta_k^\pm \mathbf{U}^{(n)} \right\|_{L_d^\infty}^2 \leq \left(\frac{1}{2L} + \frac{2^{3/4}}{2} \right) \left(\|\delta_k^{(2)} \mathbf{U}\|_{L_d^2}^2 + \|\mathbf{U}\|_{L_d^2}^2 \right).$$

Proof. We only show the case of sign + since the other case of sign - can be shown by the same fashion. From the boundary condition, $\delta_k^+ U_{-1} = \delta_k^+ U_0$ and $\delta_k^+ U_k = \delta_k^+ U_{K-1}$ hold. We obtain for any m and ℓ satisfying $0 \leq \ell < m \leq K-1$

$$|\delta_k^+ U_m|^2 - |\delta_k^+ U_\ell|^2 = 2 \sum_{k=\ell}^{m-1} \delta_k^{(2)} U_{k+1} \cdot \frac{\delta_k^+ U_{k+1} + \delta_k^+ U_k}{2} \Delta x.$$

Then for any $0 \leq \ell, m \leq K-1$

$$\begin{aligned} |\delta_k^+ U_m|^2 &\leq |\delta_k^+ U_\ell|^2 + \sum_{k=0}^{K-1} |\delta_k^{(2)} U_k| \cdot |\delta_k^+ U_k| \Delta x + \sum_{k=0}^{K-1} |\delta_k^{(2)} U_{k+1}| \cdot |\delta_k^+ U_k| \Delta x \\ &\leq |\delta_k^+ U_\ell|^2 + \left(\sum_{k=0}^{K-1} |\delta_k^{(2)} U_k|^2 \Delta x \right)^{1/2} \left(\sum_{k=0}^{K-1} |\delta_k^+ U_k|^2 \Delta x \right)^{1/2} \\ &\quad + \left(\sum_{k=0}^{K-1} |\delta_k^{(2)} U_{k+1}|^2 \Delta x \right)^{1/2} \left(\sum_{k=0}^{K-1} |\delta_k^+ U_k|^2 \Delta x \right)^{1/2} \\ &\leq |\delta_k^+ U_\ell|^2 + 2 \|\delta_k^{(2)} \mathbf{U}\|_{L_d^2} \|\mathbf{DU}\| \end{aligned}$$

holds. For fixed m , adding these through $\ell = 0, 1, \dots, K-1$ yields

$$K|\delta_k^+ U_m|^2 \leq \sum_{k=0}^{K-1} |\delta_k^+ U_k|^2 + 2K\|\delta_k^{(2)} U\|_{L_d^2} \|DU\|.$$

Then it holds that

$$\max_{m=0,1,\dots,K-1} |\delta_k^+ U_m|^2 \leq \frac{1}{L} \|DU\|^2 + 2\|\delta_k^{(2)} U\|_{L_d^2} \|DU\|. \quad (3.1)$$

Since we have

$$\sum_{k=0}^K \delta_k^{(2)} U_k \cdot U_k \Delta x = \sum_{k=0}^K \frac{|\delta_k^+ U_k|^2 + |\delta_k^- U_k|^2}{2} \Delta x = \|DU\|^2,$$

we see that

$$\|DU\|^2 \leq \|\delta_k^{(2)} U\|_{L_d^2} \|U\|_{L_d^2}.$$

Therefore, by the Young inequality, the right hand side of (3.1) is estimated by

$$\begin{aligned} & \frac{1}{L} \|\delta_k^{(2)} U\|_{L_d^2} \|U\|_{L_d^2} + 2\|\delta_k^{(2)} U\|_{L_d^2}^{3/2} \|U\|_{L_d^2}^{1/2} \\ & \leq \frac{1}{2L} \left(\|\delta_k^{(2)} U\|_{L_d^2}^2 + \|U\|_{L_d^2}^2 \right) + \frac{3^{3/4}}{2} \left(\|\delta_k^{(2)} U\|_{L_d^2}^2 + \|U\|_{L_d^2}^2 \right), \end{aligned}$$

which implies the result. \square

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